Agilent 6300 Ion Trap LC/MS Systems Quick Start Guide

A guide to help you get started with the Agilent 6300 Series Ion Trap LC/MS system

Use this document: to find help, to install and troubleshoot system hardware, to install the system software, and to acquire and analyze data with the 6300 Series Ion Trap LC/MS.

Agilent Technologies

What is the Agilent 6300 Series Ion Trap LC/MS System?

The 6300 Series Ion Trap LC/MS system consists of an Agilent LC, an atmospheric pressure ion source; and the Ion Trap mass spectrometer, which can be one of several models: 6310, 6320, 6330, and 6340.

The Ion Trap software controls the instrument and provides the tools to acquire and analyze LC/MS data. The software consists of components to help you with the following tasks:

- ChemStation—LC control, LC method development and sequence setup and execution
- 6300 Series TrapControl—Ion Trap control, MS method development, acquisition monitoring
- DataAnalysis—compound-based data-mining and -browsing, search and identification (LibraryEditor), report design (ReportDesigner) and generation, analysis automation through Visual Basic Scripting
- QuantAnalysis—quantitation

You can also obtain licenses to add on or use the program below:

- G1981AA Deconvolution and Bioanalysis Software — deconvolution of protein and peptide spectra and evaluation of MS and MS/MS data from proteins and peptides
- G3310AA Security Pack —Help for compliance with 21 CFR Part 11 regulations, including user management, audit trail, access control, electronic signatures and results revisioning

  To get started with any of the add-on software packages described above, see its *Quick Start Guide*.

Where to find additional system information

System information (hardware and software)

Manuals These manuals are available on the CDs as files in Portable Document Format (PDF).

System Installation Guide Guides you through hardware and software installation, configuring the instrument, and verifying performance, if your Agilent representative has not already done this.

System Concepts Guide Contains background information to help you understand the hardware and software and how they work together.

System Quick Reference Guide Describes reasonable starting parameter values to control the Ion Trap hardware for all modes of operation. You obtain the best performance by optimizing these settings.

Software Familiarization Guide Provides exercises to help you learn all parts of the Ion Trap software. Use this guide if a training lab is not available.

Training Courses Visit www.chem.agilent.com to view a list of training courses for the Agilent Ion Trap system.

Hardware information

User's Guide Describes the basic operation and maintenance of the Ion Trap hardware.

Software information

Online help Use online help for in-depth information not given in this *Quick Start Guide*.

Press F1 To get more information about a pane or dialog box, place the cursor on the part of the pane or dialog box of interest and press F1.

Help menu From the Help menu, access Help Topics, which includes task help, reference help and manuals online.

What's new in this release?

This section tells describes the new features in Trap Software Version 6.2.

What's new in TrapControl Software?

- PANorama fragmentation - PAN fragmentation is a newer fragmentation mode which helps overcome the 1/3 cut-off rule for Trap fragmentation. To view low mass fragments, the precursor is excited very briefly, but with a high energy. With this kind of fragmentation, the low mass fragments are retained within the trap.
- PTR/ETD - Following an ETD experiment of a large peptides, the resulting fragments can have a complicated mixture of charge states. PTR or Proton Transfer Reaction, is a charge stripping step that can significantly reduce the multiply charged fragments.
- Active Ejection - Active ejection is used in conjunction with Active Exclusion. Once an ion has been temporarily added to the Active Exclusion list, Active Ejection prevents these ions from being added to the ion population within the trap. As a result, storage of more ions not on the Active Exclusion list are allowed.
- Segment-independent Inclusion, Preferred and Exclusion Lists.

What's new in DataAnalysis Version 4.0?

- Support for PTR/ETD spectra.
- Support for PAN.

Instructional overview

1 Install the Ion Trap System hardware

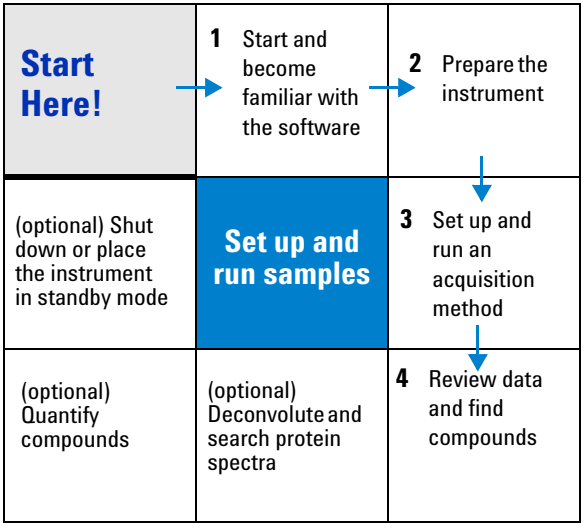
Use the instructions in the *Agilent 6300 Series Ion Trap System Installation Guide* to install the hardware.

2 Install the Ion Trap System software

Use the instructions in the *Agilent 6300 Series Ion Trap System Installation Guide* to install all the software components.

3 Set up and run samples

The roadmap below shows you the steps to set up and run a sample from start to finish. Follow the instructions on the next pages to get started and to learn where to find the information to help you with each step in this roadmap.



Step 1. Start the software

The instructions below include the following assumptions:

- The hardware and software are properly installed.
- The instrument is configured. Use instructions in the *Agilent 6300 Series Ion Trap System Installation Guide* to configure the instrument for the first time.

To start the Ion Trap software with the Security software installed, see the *G3310AA Ion Trap Security Pack Quick Start Guide*.

Start the Ion Trap software on an Ion Trap Control PC

For an online installation, the desktop displays the following icons.

Start the Ion Trap software

- Double-click the **Instrument 1 Online** icon.

  This automatically opens ChemStation, Trap Control and DataAnalysis in that order.

  You open the QuantAnalysis and ScriptStarter programs, separately.

ChemStation Controls LC, lets you save and load LC/MS acquisition methods and lets you set up and run sequences.

Trap Control Controls Ion Trap and lets you set up the MS part of a method.

Data Analysis Lets you review qualitative data and search unknowns.

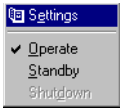
QuantAnalysis Lets you set up calibration curves and quantify compounds.

ScriptStarter Runs automated data processing for large sequences of data files, normally stored in the same directory. Automation is possible because a DataAnalysis method, which contains a script, is initially stored with an acquisition method. Then, it is transferred to the data file acquired by the acquisition method. See Chapter 3, "How LC/MS Trap Methods Work", in the *Concepts Guide* for more information on how methods are organized.

Switch between ChemStation, Trap Control and DataAnalysis

You can switch between all three programs from the Windows taskbar. Refer to the table below for instructions on how to switch to a program from within another program.

Table 1 Switch between ChemStation, Trap Control and DataAnalysis

If you want to switch to this program:	From within this program:	Do this:
Ion Trap Control	ChemStation	• Select **Method > Edit MS Method Part...**, or • Click the **Ion Trap Control** button, or 
		• Click the **MS^n** icon, and select **Settings**. 
	DataAnalysis	• Select **Tools > ChemStation**, or • Click the **Trap Control** button in DataAnalysis. 
DataAnalysis	ChemStation	• Click the **DataAnalysis** button in ChemStation. 
	Trap Control	• Click the **DataAnalysis** button in Trap Control. 
ChemStation	Trap Control	• Click the **ChemStation** button in Trap Control. 
	DataAnalysis	• Select **Tools > ChemStation**, or • Click the **ChemStation** button in DataAnalysis. 

Start the Ion Trap software for an offline installation

You use an offline installation, or standalone system, to analyze data. Therefore, the ChemStation or Trap Control programs are not installed.

For an offline installation the desktop displays the following icons.


DataAnalysis


ScriptStarter


QuantAnalysis

- Double-click any button to start the program of choice.

Open the LibraryEditor or ReportDesigner programs

Included with the DataAnalysis software, for both online and offline installations, are the LibraryEditor and ReportDesigner programs.

Open the LibraryEditor program

The LibraryEditor program lets you create spectral databases and search mass spectra of unknown compounds against those databases.

- Select **Start > Programs > Ion Trap > LibraryEditor**,

or

1. Open **DataAnalysis**.
2. Click the **LibraryEditor** button. 

Open the ReportDesigner program

The ReportDesigner program lets you create your own report layouts or modify the existing ones.

- Select **Start > Programs > Ion Trap > ReportDesigner**,

or

1. Open **DataAnalysis**.
2. Select **Print...**, or **Print Preview...**,
3. Select **ReportDesigner...**.

Step 1a. Become familiar with the software

ChemStation window

The ChemStation window is the first window that appears when you start an online system for instrument control. You use the ChemStation software to develop the LC part of LC-only or LC/MS methods, set up information for single runs or sequences and acquire data. See the *Agilent ChemStation document set* and *ChemStation Online Help* to familiarize yourself with this software.

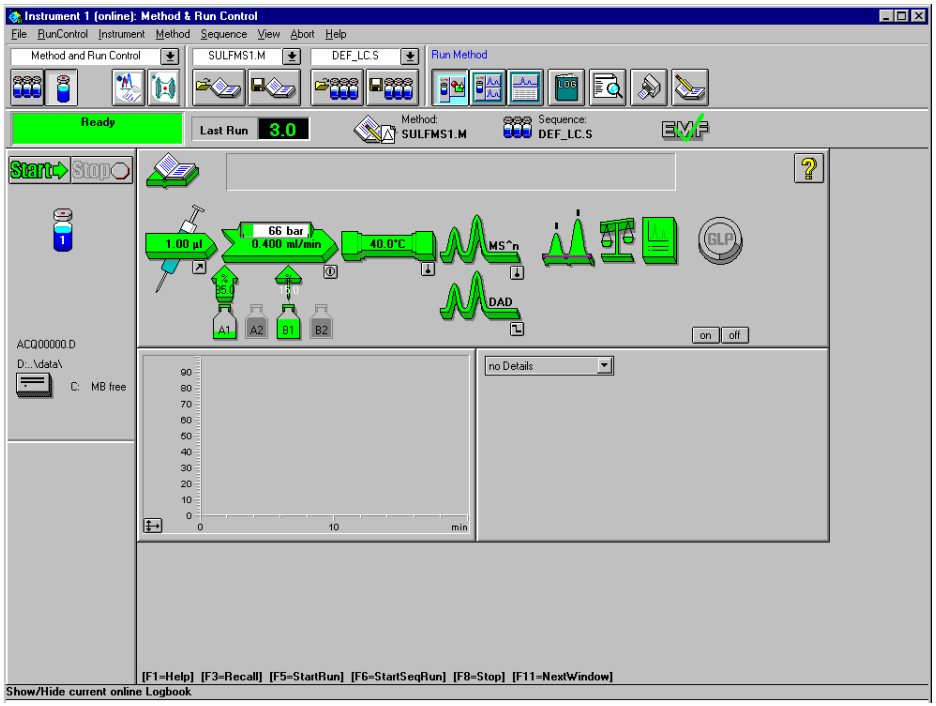


Figure 1 ChemStation window

Trap Control window

The initial (default) Ion Trap Control window contains three panes, three areas for acquisition parameter entry, and menus and a toolbar to set up and run MS acquisition. (Figure 2).

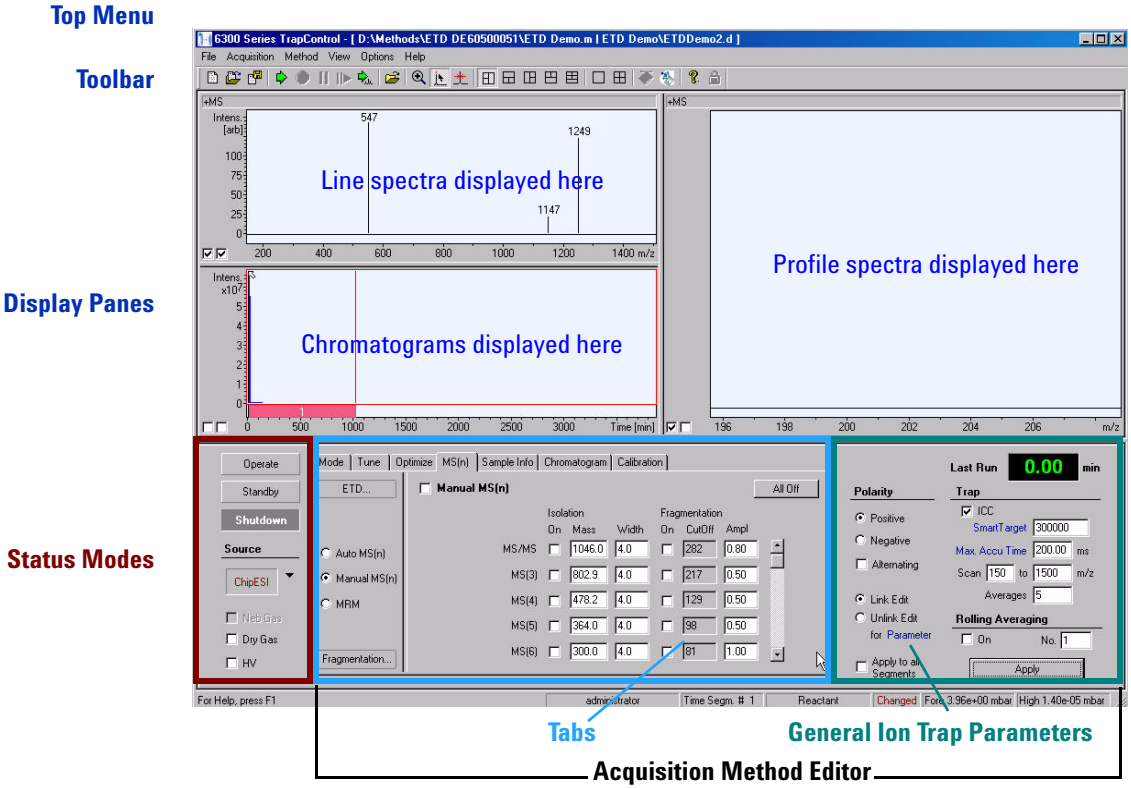


Figure 2 Initial Ion Trap Control window

Toolbar and Top Menu

The toolbar contains buttons that help you set up and run MS data acquisition. Many of the actions accessed through the Top Menu and the toolbar are the same. For menus and menu items not listed below, please refer to the Online Help.

Table 2 Actions that you can do through the Ion Trap Control toolbar and top menu

If you intend to do this:	Click this toolbar button or select this menu item from the top menu:	Additional information
Create a new MS method	Method > New - 6300 Series TrapControl Part (Ctrl+N)	• Loads Def_MS.M
Open an existing MS method	Method > Load - 6300 Series TrapControl Part (Ctrl+O)	
Save the MS method	Method > Save -6300 Series TrapControl Part (Ctrl+S)	
Start the acquisition	Acquisition > Run Method (F5)	• Acquires the data in the way prescribed by the method that is currently loaded. • Note that when you are using Trap Control to acquire MS-only data, **Run Method** acquires to the file and directory specified by Sample Info in the tab. If the MS acquisition is part of an LC/MS method run from ChemStation, then the file name and directory locations are prescribed in ChemStation's Sample Info.
Stop the acquisition	Acquisition > Stop Run (F8)	
Pause the acquisition	Acquisition > Pause (Ctrl + F8)	

If you intend to do this:	Click this toolbar button or select this menu item from the top menu:	Additional information
Continue the acquisition (after a pause)	 Acquisition > Continue (Ctrl+F5)	
Save a single profile spectrum	 Acquisition > Save Profile Now (F7)	• Acquires a single data point as a Profile spectrum to a data file. • The name of this data file and its location are prescribed in the Sample Info tab.
Zoom in	 View > Zoom in (F9)	Lets you draw a rectangle with the mouse around the area to zoom.
Select the mass with the maximum abundance to the left of the mouse cursor position.	 View > Maximum Cursor (F10)	Click this button, position the cursor and click the mouse button to do this.
Show peak width in Profile spectrum	 View > Show peak width in Profile Spectra (Ctrl+W)	
Change the arrangement of the graphics windows (panes). The first arrangement is the default partition.	 View > Arrange Spectrum Windows > 1-5	Use arrangement #5 for AutoMS(n) acquisition to see the MS spectra above and the MS/MS spectra in the middle. Drag the border of the chromatogram upward to see the middle.
Maximize the active spectrum window	 View > Maximize Spectrum Window	
Tile the spectrum windows	 View > Tile Spectrum Windows	
Show the LC program	 View > LC Program (Shift+F11)	
Show DataAnalysis Program	 View > DataAnalysis (F11)	
About Trap Control	 Help > About...	

If you intend to do this:	Click this toolbar button or select this menu item from the top menu:	Additional information
Lock all applications	 Help > Lock all Applications (Ctrl+Alt+K)	• Available only after installation of the Ion Trap Security Pack
Print or preview the chromatogram and spectrum panes	File > Print File > Print Preview	
Open an Analysis file and the method from this file	 File > Open Analysis File (Ctrl+D)	

Display panes

Line and Profile spectral panes Line spectra do not show peak widths because all of the Profile peak intensities within a range determined by the Line spectrum algorithm have been summed and grouped into a single Line spectrum peak.

- To compare Line and Profile spectra:
  - **a** Clear the right-hand check boxes in the lower left corner of each spectral pane.
  - **b** To adjust the frame border move the cursor to the edge and click and drag the border until your screen appears as in Figure 3.

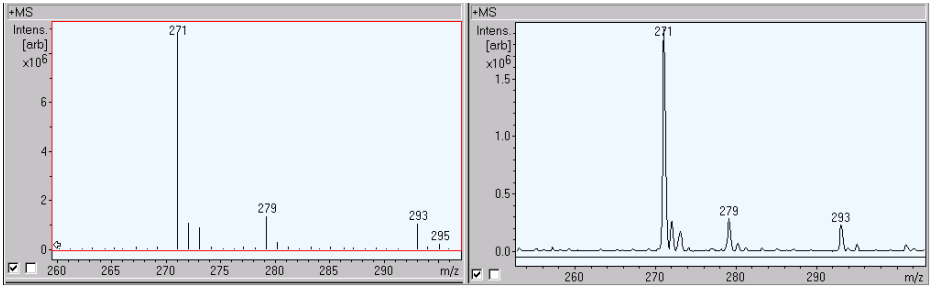


Figure 3 Comparison of a Line spectrum and Profile spectrum

- To return to the normal view:

  - Mark the right-hand check box at the lower left.
- To change the window axis range in the Profile spectrum view:
  a. Move the cursor over the axis until it changes into a bidirectional arrow
  b. Click and drag the axis to change the span of the range, or right-click and drag the range to change the sensitivity of the span.

  You cannot change the offset in the Line spectrum view.
- To enlarge different parts of the window:
  - Click the **Zoom-in** button and draw a box around the area of interest.

Shortcut menus If you right-click a display pane, you can access shortcut menus. These menus let you change the display properties of each display pane and provide other useful features. The specific content of the line spectrum menus depends upon the tab that is open. The content is the same for all the tabs except for the MS(n) view and the Chromatogram view.

Acquisition Method Editor: Tabs

The Trap Control window includes seven tabs that contain parameter fields to control and monitor operation of the Ion Trap during acquisition. To download parameters to the Ion Trap after you make changes, you click Apply.

Mode The Mode tab lets you select from three sets of parameters.

- Save Spectra—This feature lets you specify “if and which” data are acquired.
- Scan Mode—You can set the speed and resolution of a scan by selecting from different scan modes. These selections are the scan modes available for your particular instrument model (6310 or 6320).
- Divert Valve—When you are running an LC/MS method that elutes large quantities of compounds that are not of interest, you may not want to acquire MS data on them nor admit them into the ion source, which increases the frequency of cleaning. Using the time segment feature of the software, you may direct these compounds To Waste (as long as the LC is connected to the ion source through the divert valve). Also, you may turn off the Save Spectra feature in this tab for this segment, which saves disk space. See “Exercise 3. Change and run method to optimize peak height” on page 45 of the *Familiarization Guide* to learn how to set up segments.

Tune Tune tab provides two sets of parameters under the Smart Parameter Setting (SPS) and the Expert Parameter Setting (EPS).

- Smart Parameter Setting–These settings let you control the ion optics and ion trap accumulation as well as all supported sources. The default settings provide an optimum signal for the positive ions of the ESI Tuning Mix (G2431A).
- Expert Parameter Setting–Because adjustments made to the Smart Parameter Settings automatically adjust the Expert Parameter Settings, we recommend that you complete most signal optimization procedures in the Smart view.

Optimize Use this tab to change values of the ion optics, ion trap drive or fragmentation voltage, and mass product ion cutoff.

MS(n) This tab lets you enter parameters to isolate and fragment precursor ion(s), where the number of MS levels (n) varies depending on the Ion Trap model. AutoMS(n) performs multiple iterations of MS/MS on a defined number of precursor ions using generic parameters. ManualMS(n) lets you enter parameters for each product ion. MRM (Multiple Reaction Monitoring) isolates and fragments multiple precursor ions through one or two iterations.

Sample Info Enter information on the sample that you intend to run.

Chromatogram Use the Chromatogram tab to enter the information to monitor traces in the Chromatogram pane. You can also enter the chromatographic trace information when you click a line spectrum peak with the mouse maximum cursor activated.

Calibration There are two types of calibration: Automatic and manual. Automated lets you execute algorithms to complete Scan (MS-only), Isolation, or Fragmentation calibrations. To manually perform each calibration, you select a radio button.

Acquisition Method Editor: General Ion Trap Parameters

Ion Charge Control (ICC) The ICC Target (or Smart Target for 6310, 6320 and 6330 models) controls the number of ions stored in the Ion Trap on a scan-to-scan basis. If too many ions are stored in the Ion Trap, they interfere with each other's motions and are ejected from the Ion Trap at the wrong instant during the scan. This results in a slight degradation of mass assignment and resolution. Suggested values for the ICC Target are provided with the default methods (e.g., DEF_LCMS.M).

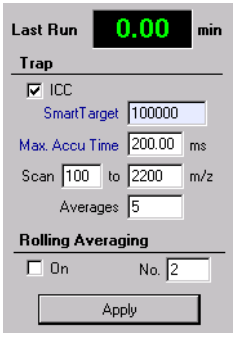


Figure 4 General MS parameters

Averages In general, the system averages and stores several scans together as a single spectrum at a designated retention time. The number of scans is controlled by **Averages** (field containing "5" in Figure 4). You can increase the number of scans to obtain cleaner-looking spectra and an improved signal-to-noise ratio. However, doing so reduces the number of data points (spectra) across the chromatographic peak as the compound elutes. Usually, for quantitative analyses the number of scans is chosen to yield 8-10 data points across the peak. For qualitative analyses, you use fewer data points (a higher number for Averages).

Rolling Averaging Rolling Averaging is a different way of averaging. For example, if Rolling Averaging is set to 2, all the scans in the previous spectrum and all the scans in the current spectrum are combined, averaged, and stored as a single spectrum at a designated retention time. This action improves the spectral quality at the expense of chromatographic fidelity. Peaks appear skewed (rapid rise followed by a longer tailing edge). Disable this feature for quantitative work.

Status Modes

Trap Control displays the current system status on the left side of the window below the spectral panes.

Operate status Green

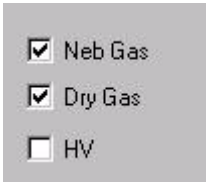
- Ion Trap is scanning and source gas settings are turned on.

Operate status Blue

- Ion Trap is scanning, source gas settings are turned on, and MS data acquisition begins.

Standby status Yellow

- Yellow—Method Standby—Source gas settings are still turned on, based on current method settings, but the voltage to all ion optics is turned off. The Ion Trap RF voltage is still on, but scanning is not in progress.

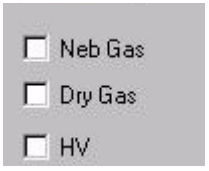


Standby status Orange

- Orange—Instrument Standby—Same as Standby Yellow except that the gas settings are those you set yourself for Standby mode, and settings are stored in the instrument so that you can shut down the software without cooling the MS down.

Shutdown status [You must shut down the Ion Trap before you are able to switch the ion sources.]

- Source gas settings are switched off, and there is no voltage to the ion optics and no scanning of the Ion Trap. The Divert Valve is switched To Waste.



DataAnalysis window

With the DataAnalysis window, you work with the raw data that you acquired with acquisition methods set-up through the ChemStation and Trap Control windows. In DataAnalysis, you can extract chromatograms, find unknown compounds, extract averaged compound mass spectra, deconvolute mass spectra and print reports.

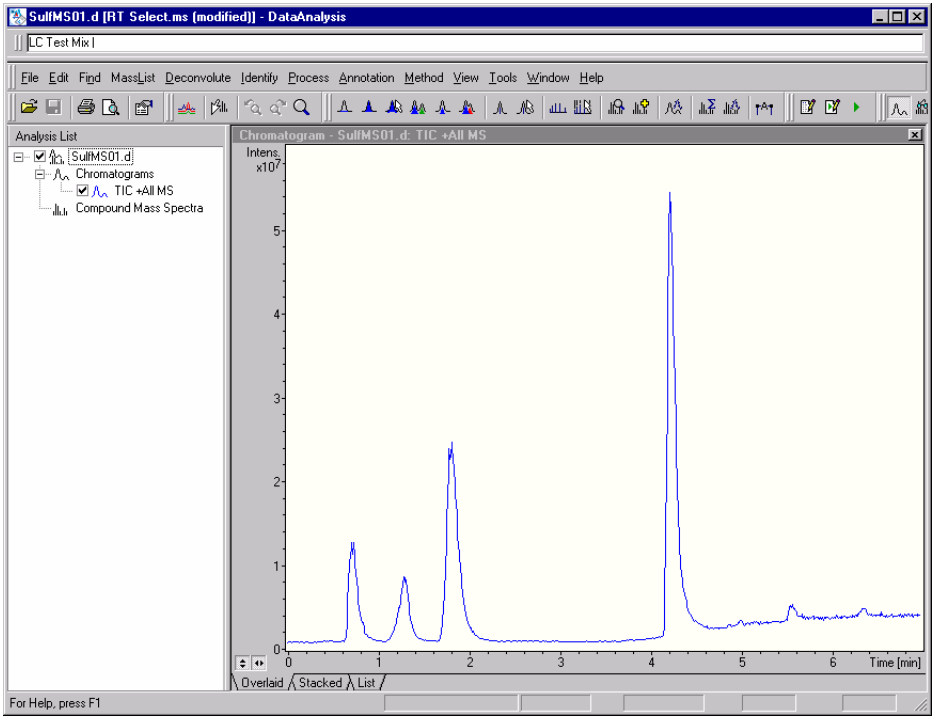


Figure 5 DataAnalysis window

See "Step 1. Start the software" on page 6 to learn how to open this window.

See "Step 4. Review data and identify compounds" on page 27 and "Deconvolute and search protein spectra" on page 34 for more information on how to use this window.

QuantAnalysis window

For most of your analyses, you probably want to review spectra and search for unknowns. You do this through the DataAnalysis window. If you intend to set up a calibration curve and quantitate target compounds of interest, you start QuantAnalysis and use the window shown below.

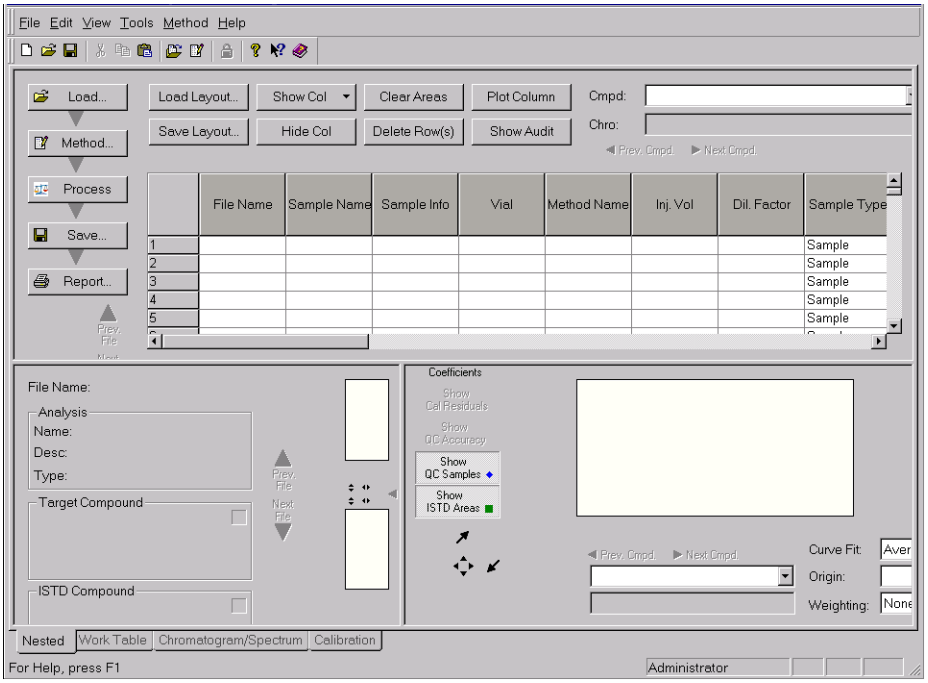


Figure 6 QuantAnalysis window

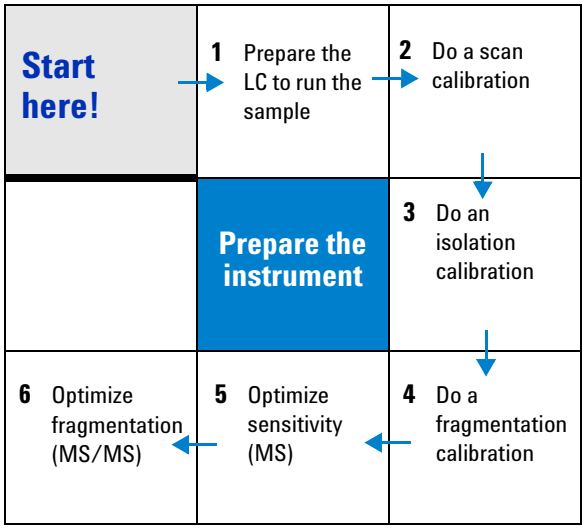
See "Step 1. Start the software" on page 6 to learn how to open this window.

See "Quantify compounds" on page 35 for more information on how to use this window.

Step 2. Prepare the instrument

Read and follow the steps in the user information listed below to learn how to prepare the instrument for a run.

- Chapter 1, “Prepare for the analysis”, in the *Familiarization Guide* to learn to prepare the LC and Ion Trap to run an ESI demo sample. This chapter includes exercises to help you learn to calibrate and tune the instrument.
- *Online Help* for the tasks listed in the roadmap below and descriptions of the fields found in the windows and dialog boxes needed for these tasks are as follows:



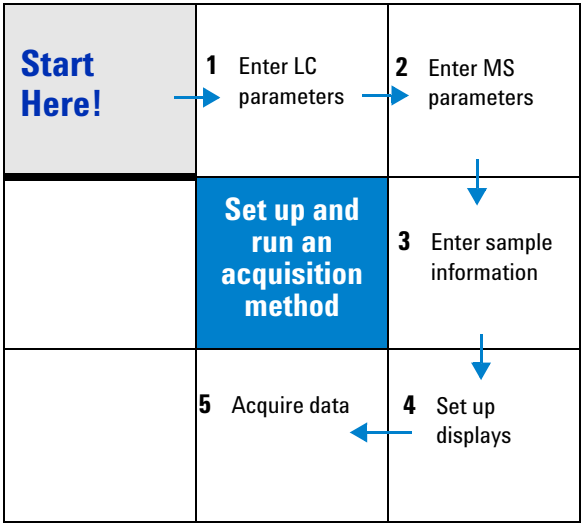
Step 3. Set up and run an acquisition method

Before you do this step, make sure that the instrument has been tuned and calibrated recently, or that the current calibration is accurate. If not, follow the instructions in Chapter 1, "Prepare for the analysis" of the *Familiarization Guide* to tune or calibrate the instrument.

Read and follow the steps on the next pages that take you through the roadmap below. These steps introduce you to the general procedure but should be used only as a quick reference. For more detailed instructions refer to the *Familiarization Guide*.

Also, refer to the user information listed below to learn how to set up methods.

- *Concepts Guide*–Chapter 3, "How LC/MS Trap Methods Work" to learn about the method and data file structure, as well as the recommended strategy for developing LC/MS methods
- *Familiarization Guide*–Chapter 2, "Set up and run acquisition methods", to learn how to perform the tasks to implement the method development strategy.
- O*nline Help* for the tasks listed in the roadmap below, descriptions of the fields in the windows and dialog boxes needed for these tasks and the tasks listed on the next pages.



Set up an acquisition method

The following procedure lists the steps you take to set up an acquisition method to run a sample mixture in positive ESI mode. To practice these instructions using an HPLC with the ESI demo sample instead, see Chapter 2, "Set up and run acquisition methods" in the *Familiarization Guide*.

Step	Detailed Instructions	Comments
1 Load the default method, DEF_LCMS.M.	a In ChemStation, to load the default method, select **Method > New LCMS method**. **b** Click **OK**. **c** Check **Status** mode to verify that the source is ESI and ion polarity is positive.	• It is recommended that you start with this default method, make desired changes and save the new method from within ChemStation.
2 Prepare the sample. • Use a test sample or the Tuning Mix in a concentration of 1 to 10 ng/ul.	• Dissolve the sample in the mobile phase used for the analysis.	• If you are setting up for quantitation, the test sample is ideally the target to be analyzed. If you are doing qualitative work, the test sample is ideally a representative of the class of compounds to be analyzed.
3 Prepare the syringe pump. • Syringe pump flow rate at 300 µl/h. (20 µl/h for nanospray) • If infusion into LC flows, set LC flow rate at 100-500 µl/min.	**a** Draw the sample into a syringe. **b** Insert the syringe into the syringe pump. **c** Connect the tubing to the nebulizer. **d** Adjust the syringe pump flow rate to 300 µl/h. (20 µl/h for nanospray). If infusing into LC flows, set LC pump rate in ChemStation.	• Be sure that no air bubbles are introduced into the syringe with the sample. • If you are performing infusion work at low flow rates, use Figure 7. • If you are infusing into LC flows, use Figure 8. • The optimal instrument parameters are determined with the actual flow rate to be used during the analysis.

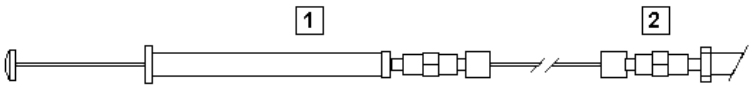
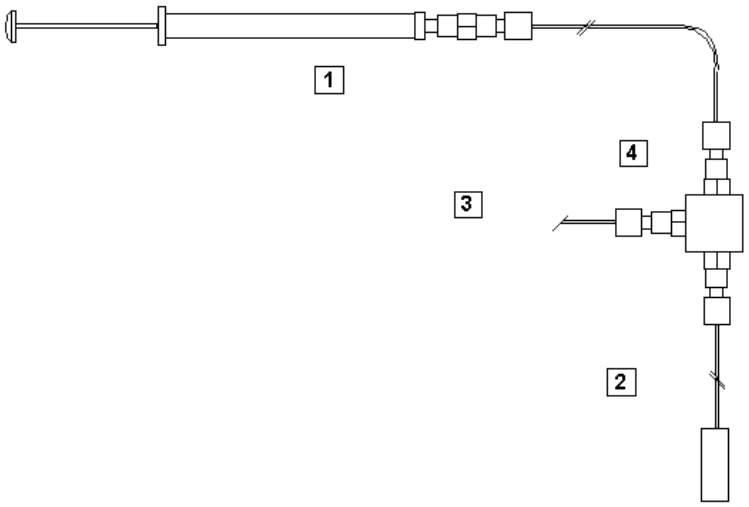


Figure 7 Tubing from the Syringe (1) to the Nebulizer (2)

Step	Detailed Instructions	Comments
		
	Figure 8 Tubing from the Syringe (1) and the LC pump (3) connected with a tee connection (4) to the effluent tubing of the Ion Trap (2)	
4 Set ion source parameters. • Smart parameters • If infusion only: Nebulizer 5 psi – 15 psi Dry Gas 5 l/min Dry Temp 325 °C • If LC + syringe pump infusion: Nebulizer 20 psi – 40 psi Dry Gas 8 – 10 l/min Dry Temp 325 – 350 °C	**a** In the Trap Control window, click the **Tune** tab. **b** In Tune tab, select **Smart**. **c** Enter the values for your type of infusion.	• If you select the **Expert** option, you need to have more information about the instrument parameters. • Refer to the *Quick Reference Guide* for details.
5 Switch to Operate state.	• On the Main window, select the **Operate** button.	• All of the electrical elements for generating and directing ions are turned on.

Step	Detailed Instructions	Comments
6 Start the flow.	• Switch on the flow of the syringe pump (and the LC pump, if necessary).	• Let the Nebulizer Gas, the Dry Gas, and the Dry Temp reach the set values. • The capillary current should read more than 25 nA, indicating an adequate spray of ions.
7 Set the desired target mass.	**a** Set the value using the Smart Parameter Setting (SPS) accessed from the Smart Tune tab. **b** You can enter the target mass: • manually from your keyboard. • with the mouse wheel (increase steps with or without holding the Shift or Ctrl key). • from the Line spectrum window– activate the mouse cursor, click beside the peak, then right click to access a shortcut menu, and select **Run SPS**.	• Typically, the SPS Target is set to the molecular ion mass of interest, or in the middle of the mass range for a distribution of ion masses in a sample mixture.
8 Save a method.	**a** Click **Method > Save Method As...** **b** Replace the name of the default method with the name of your new method. **c** Click **OK**.	• You cannot change the name of the default method. You must save all changes under a new method name.

Acquire MS/MS spectral data only

Step	Detailed Instructions	Comments
1 Enter sample information.	In the **Sample Info** tab **a** In the Data File field, choose **Prefix/Counter**, and type a prefix and counter for the file name, and a new subdirectory name. **b** In the **Sample Parameter** field, you can describe the sample under Comment, and enter a **Sample Name**, if desired. **c** To accept the information click **Apply**.	• You must enter the information if you run a method directly from within Trap Control without first starting in ChemStation. • The Comment and Sample Name, if defined, are displayed in the Ion Trap DataAnalysis program in the Analysis Info window during Post-processing.
2 Turn on isolation and fragmentation.	**a** Open the MS(n) tab and check the **Manual MS(n)** check box. **b** Enable the Maximum Cursor Tool: • Use the Maximum Cursor button, • Use the F10 shortcut, *or* • From the toolbar, click **View > Maximum Cursor**.	
3 Select an ion to fragment.	**a** In the Line Spectrum window, click to the right of the peak of interest. **b** Enter the isolation mass with an isolation width of 4 mass units. **c** Right-click in the Line Spectrum window to open a shortcut menu, and select **Isolate/Fragment**.	• This centers the mass of the peak of interest in the Mass window. • The previously selected mass is set as the isolation mass. • Check that the ion is isolated and all other ions in the Line Spectrum window disappear.
4 Optimize the spectrum by setting the Fragmentation Amplitude.	a Increase or decrease the amplitude in increments of 0.1 until the isolated ion is reduced to about 10% of the initial intensity, and the fragment ions are present in significant amounts. **b** Enter a new amplitude with: • the keyboard, • scroll-bar buttons, *or* • the mouse wheel.	

Step	Detailed Instructions	Comments

5 Save the mass spectrum.	• Save the desired mass spectra:
	  • Click the **Save a single profile** toolbar button, *or*
	  • Press the **F7** key, *or*
	  • From the top menu, click **Acquisition > Save Profile Now**.
		• The saved file is named test0000.d.

6 Isolate and fragment another mass.	• Repeat Steps 3-5.	• The saved file is named test0001.d.
7 Turn off isolation and fragmentation.	• In the MS(n) tab, select **Manual MS(n) > All Off**.	

Acquire chromatographic and spectral data

Steps	Detailed Instructions	Comments

1 Start an acquisition to acquire chromatogram data.	Start the acquisition in ChemStation:
	  • Click the **Start** button, *or*
	  • From the top menu, select **RunControl > Run Method** *or* **Run Sequence**.
		• Make sure that the LC settings are correct.
		• Assume that you have entered the appropriate sample information and data file name into the Sample Info tab.

2 Stop the acquisition.	Stop the method manually:
	  • Click the **Stop** button, *or*
	  • From the top menu, select **RunControl > Stop Run**.	

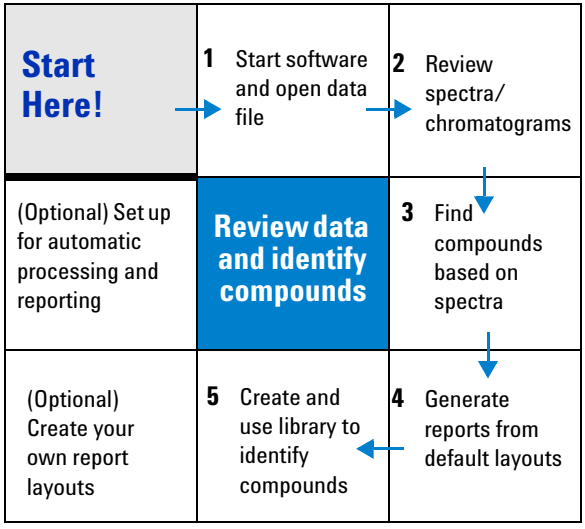
Step 4. Review data and identify compounds

The primary tool for analyzing and reporting on results is the DataAnalysis software.

Read and follow the steps on the next pages that take you through the roadmap below. Use these steps only as a quick reference. For more detailed instructions, refer to the *Familiarization Guide*.

Also, refer to the user information listed below to learn how to review Ion Trap data, generate reports, identify compounds with library search and set up automation.

- *Concepts Guide*–Chapter 1, "Comma Separated Value (CSV) Methods for Ion Trap Control", to help you understand the data file structure and what goes on behind the scenes during processing.
- *Familiarization Guide*–Chapter 3, "Review data and identify compounds", to help you learn how to use data processing methods to set up report automation, as well as how to review data and identify compounds.
- O*nline Help* for the tasks listed for the roadmap below and descriptions of the fields found on the windows and dialog boxes needed for these tasks.



Start the DataAnalysis software

If you want to do this:	Follow these instructions	Notes
Start the software.	• Click the **Data Analysis** button to display the main window.	
Open a data file.	**a** Select **File > Open**. **b** Select the file (e.g., SulfMS01.d) **c** Click **Open**.	

Review chromatograms and spectra

If you want to do this:	Follow these instructions:	Notes
Display an extracted ion chromatogram (EIC) in Data Analysis.	**a** Click **Edit > Chromatograms...** to display the dialog box. **b** Select **Type > Extracted Ion Chromatogram**. **c** Select filter: All, MS, MS2 or... (as desired) **d** Enter desired value in Masses field. **e** Click **Add** to add the trace to the list.	• You can also use the **F7** keyboard shortcut to access this dialog box. • Use a single value to specify a single mass +/- the width value. Use a "-"separator (298.5-303.5) to specify a range, and use a ";" separator (274;281) to specify the sum of two masses.
Change the properties of an existing trace.	a Click **Edit > Chromatograms...** to open the dialog box. **b** Select the trace with the mouse cursor. **c** Make the desired changes. **d** Click **Change** to confirm the changes to the trace. **e** Click **OK**.	

If you want to do this:	Follow these instructions:	Notes
Create an averaged spectrum.	**a** Check that the **Select Range / View Spectra** tool bar button is not selected. **b** Click on a peak and drag the cursor over it to select a range of spectra in the chromatogram. **c** Click the **Average** tool bar button to get an average of the spectra across the peak. **d** Click the **Select Range/View Spectra** button to activate View Spectra.	• When the button is not depressed, **Select Range** is selected, and the cursor is arrow-shaped. • When this button is depressed, **View Spectra** is selected, and the cursor appears as an arrow next to a spectrum that resembles the Tool button, itself.
Check for possible changes in the Line and Profile displays of the Mass Spectrum view.	**a** Select **Tools > Options > Mass Spectrum View > Spectrum Type.** **b** Select **Line** or **Profile**.	• You can view both Centroid (Line) and Profile spectra, only if you specify Profile data acquisition.
Select a single point mass spectrum in the Mass Spectrum view.	• Click anywhere on the chromatogram.	

Find compound MS spectra

If you want to do this:	Follow these instructions:	Notes
Find compound spectra.	**a** Make sure that **Select Range** is activated (button deselected). **b** Click and drag the cursor over the desired area. **c** Select **Find > Parameters**. **d** Click the **Chromatogram, MS(n)** tab. **e** From the **Spectrum Type** list, select **Line and profile spectra**. **f** Select **Find > Compounds – Chromatogram.**	• This algorithm locates the peaks in the MS chromatogram, integrates those peaks, averages the mass spectra under those peaks, and transfers the averaged mass spectra to the Compound Mass Spectra window. • This function applies to a selected MS chromatogram.
View three spectra in the same window.	**a** Right-click the **Compound Mass Spectra** window. **b** Select **List windows > 3 windows**.	

If you want to do this:	Follow these instructions:	Notes
Review the compound integration results in the Compound List.	• Select **Windows > Compound List**.	
Change the display of the Compound List.	**a** Right-click the **Compound List** window. **b** Select **Layout**. **c** Click one or more of the tool buttons to change the layout of the list. **d** Click **OK**.	• Use tool buttons to the right of the Compound List Layout label to add, subtract or change the order of the results.

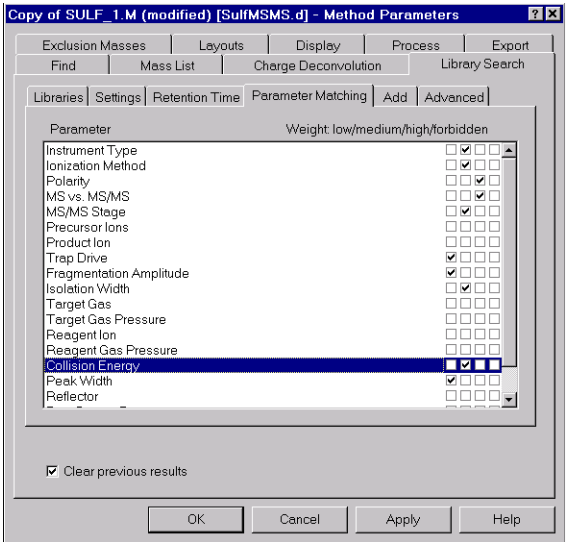
Find compound MS/MS spectra and generate a results report

If you want to do this:	Follow these instructions:	Notes
Automatically generate extracted ion chromatograms and mass spectral results for a data file acquired using AutoMS(n), (e.g., SulfMSMS.d).	• Select **Find > Compounds – AutoMS(n).**	• This performs the following analytical steps: ◦ Finds the MS2 experiments. ◦ Generates EICs with MSn filters. ◦ Averages all MS2 spectra from the same parent. ◦ Averages all preceding MS spectra. ◦ Transfers all spectra to mass spectral results. • The results of the Find operation are listed in the Analysis List window. • This function applies to the entire analysis and not to a specific chromatogram.
Print a Compound Mass Spectrum Report.	**a** Select **File > Print...** **b** For this example, select **Cmpd Mass Spec Report –AutoMS(n) (P)** from the list of Layouts. **c** Click **OK**. **d** When prompted to save your processed results, always click **Yes.**	

Create and use a library to identify unknowns

If you want to do this:	Follow these instructions:	Notes
Create a new library database.	**a** From DataAnalysis, click the **Library Editor** button. The Library Editor program opens.  **b** Click **File > New**. **c** Navigate to the folder intended to hold this library. **d** Enter the name of the library. **e** Click **Save**, then select **File > Close**.	• Each library must be placed in a separate folder, because the data files generated during library setup have identical names for all libraries created. • For convenience, give the folder the same name as the library database.
Add the MS and MS/MS spectra of a compound to the library.	**a** Open the data file upon which you intend to base your library. **b** Find the compound spectra. **c** Select the MS spectrum of a compound in the Analysis List. **d** Select **Identify > Add to Library.** **e** Enter the compound name for the spectrum. **f** Click **OK** to enter the MS spectrum. **g** Repeat **steps c-e** above with the MS/MS spectrum of the compound.	
Select the library database you created earlier to search against.	**a** Open another data file and find the compound spectra. **b** Select **Identify > Parameters...**. **c** Click the **Libraries** tab. **d** Click the **New** (Insert) button in the Libraries tab.  **e** Click the **Browse** button (...). **f** Select the database, and click **Open**.	

If you want to do this:	Follow these instructions:	Notes
Specify additional search parameter weighing factors, as in the figure below. (Typically, you would start with the default parameters.)	**a** Click the **Parameter Matching** tab. **b** Mark the appropriate check boxes and click **OK**.	• You must specify these parameters in the library database to be able to use them.
Identify the new mass spectra.	**a** Select the mass spectra in the Analysis List. **b** Select **Identify > Mass Spectra.**	• The library searches every highlighted spectrum in the Analysis List of a single data file. To limit the identification of spectra using a library database, select only the spectra that are of interest.



If you want to do this:	Follow these instructions:	Notes
Review the results of the Library search in the Compound List.	**a** Select **Window > Compound List.** **b** Right-click on the **Compound List** window and select **Layout...** from the menu. **c** Click the **Layouts** tab. **d** Click the **Compound List Layout** tab. **e** Add the parameters you want to view in the Compound List. **f** Click **OK**.	
Print the results from the Compound List window to a Library Search Report.	**a** In DataAnalysis, select **File > Print....** **b** Select **Library Search Report – AutoMS(n)** from the pull-down list. **c** Click **OK**.	

Optional steps

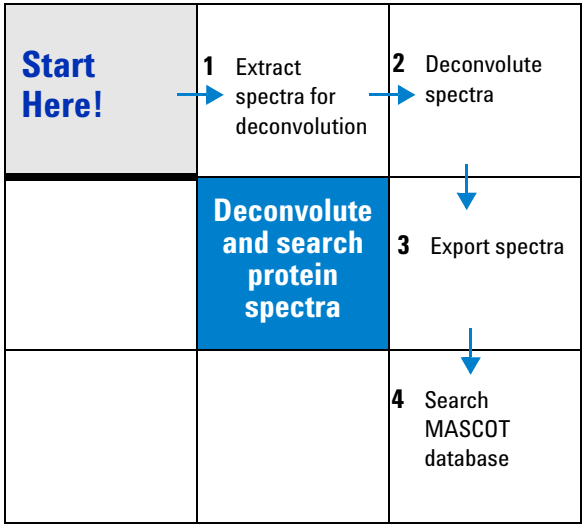
Deconvolute and search protein spectra

You can search databases such as MASCOT to identify proteins and peptide mixtures resulting from the digestion of proteins. To search MASCOT you must export *deconvoluted* profile spectra.

Deconvolution is the calculation of protein or peptide molecular weights from ions that exist in multiple charge states.

Read and follow the steps in the user information listed below to learn how to deconvolute mass spectra, export the spectra to a MASCOT Generic File (MGF) and search MASCOT to identify the protein or protein digest from its spectra.

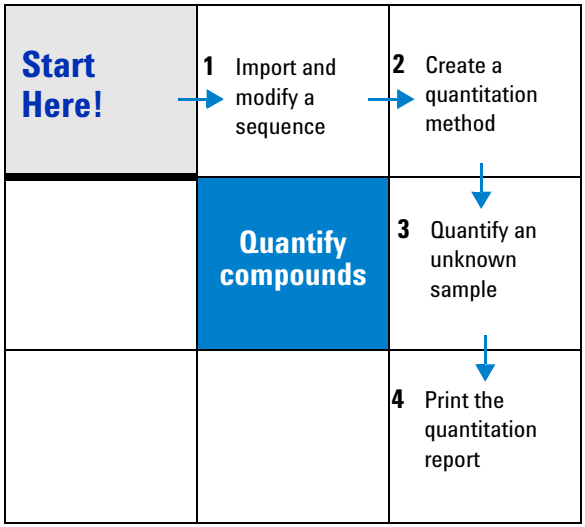
- *Familiarization Guide*—Chapter 4, "Deconvolute and search protein spectra"
- *Online Help* for the tasks listed for the roadmap below and descriptions of the fields found in the windows and dialog boxes needed for these tasks.



Quantify compounds

Read and follow the steps in the user information listed below to learn how to perform single- and multi-component quantitative analyses on data files containing calibration standards, quality controls (QCs), and unknown samples.

- *Familiarization Guide*—Chapter 5, "Quantify compounds"
- O*nline Help* for the tasks listed for the roadmap below and descriptions of the fields found on the windows and dialog boxes needed for these tasks.



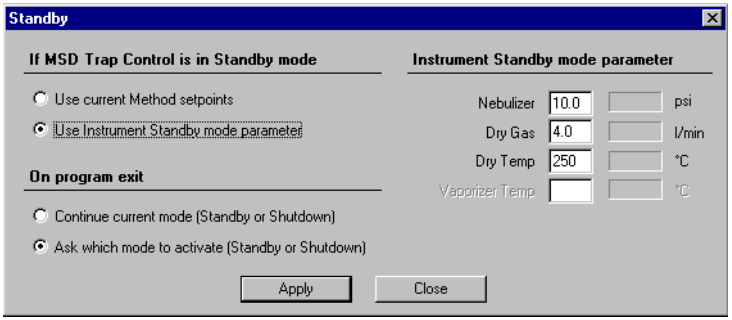
Shut down or place the instrument in Standby Mode

To learn the distinctions between the Standby and Shutdown modes, see "Status Modes" on page 17. For more details on this task see the *User's Guide*.

Place the instrument in Standby mode

Place the Ion Trap in Standby, when it is not in use.

1 From the Trap Control window, select **Options > Standby**.



2 To use the source setpoints that are in the currently loaded method when the instrument goes into Standby, select **Use current Method setpoints** (yellow), or
To use source setpoints that you enter yourself, select **Use Instrument Standby mode parameter** and enter values on the right of the dialog box. (orange)

Note that if you close the TrapControl software when the system is in Method Standby (yellow), the MS cools down, and solvent waste can be sucked into the vacuum system. This does not happen in Instrument Standby mode because the gas parameter values are stored in the instrument.

Make sure that the gas pressure and flow values are no lower than the following values and the temperature value is no higher than the following value:

- Nebulizer Pressure = 5psi
- Dry Gas Flow = 3 l/min
- Dry Gas Temperature = 300C

3 Select **Ask which mode to activate**, and click **Apply**.

4 Exit the TrapControl software.

5 When the message appears to ask for Standby or Shutdown, select **Standby**, and click **OK**.

Place the instrument in Standby mode at the end of a sequence

- In the ChemStation window, type “macro SHUTDOWN.MAC,go” in the command line, or

  Select **Sequence > Sequence Parameters** and enter the macro as a Post-Sequence Cmd/Macro.

When the sequence ends, the macro performs the following actions:

a Turns off the LC pump, column compartment and UV detector in Chemstation,

b Places the Trap Control in “Standby,” and

c Loads the MS-only method Standby.M into Trap Control.

The default method places the divert valve “To Waste” and sets the source settings, to conserve gas, to the same settings as listed on the previous page.

Shut down the Ion Trap instrument

Under only two conditions do you shut down the system:

- If you need to switch sources or perform maintenance that requires shutdown
- If you do not use the instrument for an extended period of time (e.g. holiday)

1. From the Trap Control window, select **Options > Standby**.
2. Select **Ask which mode to activate**, and click **Apply**.
3. Exit the TrapControl software.
4. When the message appears to ask for Standby or Shutdown, select **Shutdown**, and click **OK**.
5. Power off the instrument.
   - Close the ballast valve on the rough pump to reduce stress on the anti-suck valve.
   - Place a cover over the spray shield to reduce infusion of ambient air moisture.
   - Turn off the Ion Trap.

The system automatically shuts down in the following situations:

- Power failure to the PC or to the Ion Trap (Upon power restoration, the instrument remains shut down.)
- Gas flow error

  a Shutdown mode indicator becomes red.

  b Active run or sequence is stopped.

  c Divert valve is set **To Waste.**
- Vacuum fault

Agilent methods, data files and report layouts

DataAnalysis methods (VB Scripts and commands) and data

Table of DataAnalysis methods and test data

Automation methods come in the form of scripts and are installed with the Ion Trap software. You can add a script with the MS part of the method. These scripts automatically execute after the run if you select to run the script with the method.

You can use some of the scripts listed here as is. Others contain pieces of example code that show how the different commands are implemented. You can create your own custom script by combining and modifying these pieces of example code.

The scripts are also attached to sample data files. You can execute the scripts after loading the data file with Method > Run.

VB Scripts	Description	Test Data
Add_AllChro.M	Test AddChromatograms method.	Add_Chro.d
Add_Chros.M	Add chromatogram traces, execute "Find Compounds - Chromatogram", export the compound list, save the results and print a report.	SulfMS01.d*
Add_CNL.M	Add constant neutral loss chromatogram.	Add_CNL.d
Add_EIC_2.M	Demonstrate all properties of extracted ion chromatograms.	Add_EIC.d
Add_EIC_ions.M	Create, integrate, and print results of a summed EIC of four target masses.	SulfMS01.d*
Add_EICs.M	Create, integrate, and print results of four generated EICs.	SulfMS01.d*
Add_MPC.M	Demonstrate all properties of mass position chromatograms.	Add_MPC.d
Add_TIC.M	Demonstrate all properties of total ion chromatograms.	Add_TIC.d
Add_UV.M	Demonstrate all properties of UV chromatograms.	Add_UV.d
Add_Var.M	Demonstrate all properties of acquisition parameter traces.	Add_VAR.d
Add_Mult.M	Create an array of chromatograms.	Add_Mult.d
Add_Range.M	Demonstrate the 'AddRangeSelection' and 'AverageMassSpectrum' methods.	RangeAvg.d

VB Scripts	Description	Test Data
Auto_CDFexp.M	Create TIC and automatically exports to NetCDF format in same data file directory.	SulfMS01.d*
Auto_CSexp.M	Create TIC and automatically exports to Ion Trap ChemStation format in same data file directory.	SulfMS01.d*
Auto_LibSearch.M	Run Find Compounds - AutoMS(n) and searches spectra against specified library database.	LCDemo02.d*
Auto_MIS.M	Perform Find Compounds - AutoMS(n), deconvolution and export to MASCOT *.mgf file.	Mb-78 - AutoMS(n).d*
Auto_MIS_MgfExport.M	Works like Auto_MIS.M but exports to mgf file with same name as analysis filename (*.d)	Mb-78 - AutoMS(n).d*
Auto_MSDExport.M	Exports chromatogram to Ion Trap ChemStation data file while preserving data file name	SulfMS01.d*
Auto_PMF.M	Performs Find Compounds - Chromatogram on BPC (MS only), deconvolution and export to MASCOT *.mgf file	Mb-78 - AutoMS(n).d*
Auto_Print.M	Prints display report and includes information on running as part of acquisition	All
Decon_Single_MS.M	Performs deconvolution in Mass Spectrum window, exports to *.mgf, prints results	Cytc_000.d*
ExpMList.M	Exports mass list from Compound Mass List	ExpMList.d
ExpSpec.M	Exports spectrum from Mass Spectrum window.	Cytc_000.d*
For_All_Analyses.M	Performs analysis on all files open in DataAnalysis.	Quant data files*
Form.M	Manipulate appearance of script forms.	Dummy.d
Manual_CSexp.M	Creates TIC and exports to Ion Trap ChemStation format to user-defined directory.	SulfMS01.d*
Metabolite_ID.M	Interactive script, integrate peaks of EICs is specified by user.	SulfMS01.d*
NoiseCal.M	Calculates the noise in a pre-defined time range.	NoiseCal.d
Open_File.M	Opens another data file Add_BPC.d.	Base.d
RngeSelDiss.M	Runs the Find Compounds Dissect function for a specified time range.	S_MS.d
RngeSelAutoMSn.M	Runs the Find Compounds AutoMSn function for a specified time range.	S_AMS2N1.d

VB Scripts	Description	Test Data
Smooth_MS.M	Creates and smooths chromatogram, finds and exports compounds.	Caf01010.d
SN_Analysis.M	Checks out instrument sensitivity.	Default3.d

* Data files are used with Familiarization Guide and located on the 6.2 software CD under Guides\Example Data.

VBScript commands used in DataAnalysis methods

This table lists the VB script commands that are used in sample scripts to carry out specific tasks. Look at the VB scripts listed in the middle column to learn how the command is used.

VB Script command:	Used in these script:s:	To do this task:
AddChromatogram	Add_AllChro; Add_Chros; Add_CNL; Add_EIC_2; Add_EIC_ions; Add_EICs; Add_MPC; Add_Mult; Add_Range; Add_TIC; Add_UV; Add_Var; Auto_CDFExp; Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; Auto_MSDExport; Auto_PMF; ExpMList; For_All_Analyses; Form; Metabolite_ID; NoiseCal; RngeSelAutoMSn; RngeSelDiss; Smooth; SN_Analysis	Creates chromatographic traces like total ion Current (TIC), extracted ion current (EIC), base peak chromatogram (BPC), mass peak chromatogram (MPC), constant neutral loss (CNL), variable wavelength (VAR), UV, or UV chromatograms from DAD (UV2D).
AddRangeSelection	Add_Range; ExpMList; NoiseCal; RngeSelAutoMSn; RngeSelDiss; SN_Analysis;	Selects a user-defined retention time window (Select Range) in a chromatogram to limit further processing to only that window.
AverageMassSpectrum	Add_Range; ExpMList	Calculates the average spectrum of the selected range of a Chromatogram and creates a new Compound Mass Spectra entry with the averaged spectrum.
BaseLineSubtract	Add_Range	Performs a baseline subtraction on spectra of a Compound Mass Spectra object. The parameters for this algorithm will be taken from method.

VB Script command:	Used in these script:s:	To do this task:
Clear	Add_AllChro; Add_Chros; Add_CNL; Add_EIC_2; Add_EIC_ions; Add_EICs; Add_MPC; Add_Mult; Add_Range; Add_TIC; Add_UV; Add_Var; Auto_CDFExp; Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; Auto_MSDExport; Auto_PMF; Auto_Print; Decon_Single_MS; ExpMList; ExpSpec; For_All_Analyses; Form; Metabolite_ID; NoiseCal; Open_File; RngeSelAutoMSn; Rnge	Clears previously processed results.
ClearRangeSelections	Add_Range; SN_Analysis	Clears or removes the chromatogram range selections of AddRangeSelection.
ClearResults	Add_AllChro; Add_CNL; Add_EIC_2; Add_MPC; Add_Mult; Add_Range; Add_TIC; Add_UV; Add_Var; Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; Auto_MSDExport; Auto_PMF; ExpMList; NoiseCal; RngeSelAutoMSn; RngeSelDiss	Clears or removes the previously processed results.
Close	Add_AllChro; Add_Chros; Add_CNL; Add_EIC_ions; Add_EICs; Add_MPC; Add_Mult; Add_Range; Add_TIC; Add_UV; Add_Var; Auto_CDFExp; Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; Auto_PMF; Auto_Print; Decon_Single_MS; ExpMList; ExpSpec; For_All_Analyses; Form; NoiseCal; Open_File; RngeSelAutoMSn; RngeSelDiss; Smooth_MS; SN_Analysis	Closes the Script form if it is run manually from DataAnalysis.
Deconvolute	Auto_MIS; Auto_MIS_MgfExport; Auto_PMF; Decon_Single_MS	Same as Deconvolute | Mass Spectra. Deconvolutes Compound MS entries as well as time-independent spectra entries in the Mass Spectrum window.
Export	Add_Chros; Auto_CDFExp; Auto_MIS; Auto_MIS_MgfExport; Auto_MSDExport; Auto_PMF; Decon_Single_MS; ExpMList; ExpSpec; Form; Metabolite_ID; Smooth	Exports Ion Trap data file chromatograms to Ion Trap ChemStation, ASCII, or Net CDF formats. Also exports spectra to MGF, ASCII, XML, or CSV formats and Compound MS to MGF, XML, and CSV formats.
ExportMassList	ExpMList	Exports Compound MS mass lists to ASCII or CSV formats.

VB Script command:	Used in these script:s:	To do this task:
FindAutoMSn	Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; ExpMList; RngeSelAutoMSn	Same as Find | Compounds – AutoMS(n). Data mining for AutoMS(n) acquired data files. Creates all MS/MS traces, finds peaks in those traces, averages the product ion spectra within those peaks and adds them as Compound MS, along with their corresponding precursor ion spectra, also averaged.
FindCompounds	Add_Chros; Auto_PMF; NoiseCal	Same as Find | Compounds – Chromatogram. Data mining for MS data files. Finds all peaks in the MS chromatogram, averages the spectra in those peaks and adds them as Compound MS.
FindDissect	RngeSelDiss	Same as Find | Compounds – Dissect. Requires Dissect license option and applies only to MS chromatograms for trace analysis. Analyzes all possible EIC to determine if any peaks exist within the limitations set in the corresponding Method Properties of Dissect. It then generates peaks with Compound MS spectra.
FindMSn	Add_Range	Same as Find | Compounds – MS(n). Data Mining of ManualMS(n) and MRM data files. Generates all MS/MS chromatograms, finds peaks within those traces, averages the spectra under those peaks, and adds them as Compound MS entries.
Identify	Auto_LibSearch; ExpMList	Same as Identify | Mass Spectra. Finds compound mass spectra matches with library database(s) specified in Method Parameters.
IntegrateOnly	Add_EIC_ions; Add_EICs; Metabolite_ID; Smooth; SN_Analysis	Same as Find | Integrate Only – Chromatogram. Data Mining of MS and UV data files. Finds peaks within the chromatograms traces and integrates them. Places results in Compound List.
Open	Open_File	Opens *.d file from user-specified directory.
Print	Add_Chros; Add_EIC_ions; Add_EICs; Auto_LibSearch; Auto_MIS; Auto_PMF; Auto_Print; Decon_Single_MS; Smooth; SN_Analysis	Prints processed results to report layouts as applicable.

VB Script command:	Used in these script:s:	To do this task:
Save	Add_Chros; Add_EIC_ions; Add_EICs; Auto_LibSearch; Auto_MIS; Auto_MIS_MgfExport; Auto_MSDExport; Auto_PMF; Decon_Single_MS; Metabolite_ID	Saves results to Analysis file on hard drive.
Smooth	ExpMList; Smooth; SN_Analysis	Smooths chromatograms or profile spectra.

VBScripts References and Tools

OnLine Help

- To access detailed information concerning the VBScript commands specific to the Ion Trap DataAnalysis software, select **Help > Help Topics > Contents > Reference > Automating tasks in DataAnalysis.**

VBScript Language

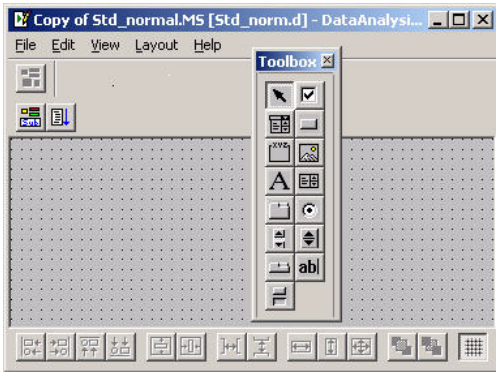
- For details concerning the general use of the VBScript language, select **Help > VBScript on the Web > Install VBScript Language Reference...** in DataAnalysis.

  A connection to the Internet is required to complete this installation.

ActiveX Controls

- To activate interactive tools for use with the VBScripts in Ion Trap DataAnalysis, select **Help > VBScript on the Web > Install Microsoft ActiveX Control Pad...**

  This enables the use of a special toolbox for use in the Object View of the VBScript window (see figure below).



Comma Separated Value (CSV) Methods for Trap Control

These methods are located on the 6.2 software CD-ROM under CSV Methods for Trap Control and are not installed with the Ion Trap software. They have a special CSV format and can be loaded to overwrite one or several parameters in an Trap Control method section. These methods are not commonly used and are intended for future customization of the software by software developers.

CSV Methods	Description
All Inst 5SegmentsSaveSpectra	Defines a Method with five segments to specify the different ways to acquire data.
All Inst SPS822	Defines a Method with only one Segment.
CL OneSegmentMRM(3)_2Ions	Defines a Method with only one Segment and MRM operations.
CL_SL_XCT NegativeAndManualMSn	Defines a Method with only one Segment and MS/MS operations.
CL_SL_XCT OneSegmentAutoMSn	Defines a Method with only one Segment and Auto MS(n) operations.
CL_SL_XCT OneSegmentManualMS(4)	Defines a Method with only one Segment and MS/MS operations.
SL_XCT 3Segment	Defines a Method with only three Segment operations.
SL_XCT 4Segments	Defines a Method with four Segments.
SL_XCT OneSegmentMRM(3)_2Ions	Defines a Method with only one Segment, MRM operations and three iterations of two precursor ions.
SL_XCT Options	Options and Advanced dialogs.

Report Layouts for DataAnalysis and QuantAnalysis

These layouts are installed with the Ion Trap software. You select one of these layouts prior to printing. If you need to modify a layout with the ReportDesigner, the layouts are located in C:\BDALSystemData\Report Layouts directory.

DataAnalysis	Description
! Print Me 1st. layout	Contains important information concerning printer support (also available in QuantAnalysis).
Acq Parms Report - AutoMSn (P)*.layout*	Instrument acquisition parameters, which include AutoMS(n) settings and ion optics parameters for the 6310, 6320 and 6330 models.
Acq Parms Report - MS (P).layout	Instrument acquisition parameters, which include MS settings and ion optics parameters for the 6310, 6320 and 6330 models.
Acq Parms Report - MSn (P).layout	Instrument acquisition parameters, which include MS(n) settings and ion optics parameters for the 6310, 6320 and 6330 models.
Cmpd chrom Report 3R1C - MS (P).layout	Analysis Info contains most important acquisition parameters, Compound List table, and individual traces displayed in a 3 row, 1 column per page format.
Cmpd chrom Report 4R1C - MS (P).layout	Analysis Info contains most important acquisition parameters, Compound List table, and individual traces displayed in a 4 row, 1 column per page format.
Cmpd Mass Spec List Report - MS (P).layout	Analysis Info contains most important acquisition parameters, chromatogram display (overlaid), compound mass spectra and corresponding mass lists.
Cmpd Mass Spec Report - AutoMSn (P).layout	Analysis Info contains most important acquisition parameters (including AutoMS(n)), chromatogram display (overlaid) and compound mass spectra
Cmpd Mass Spec Report - MS (P).layout	Analysis Info contains most important acquisition parameters, chromatogram display (overlaid) and compound mass spectra
Cmpd MS Decon Report - AutoMSn (P).layout	Analysis Info contains most important acquisition parameters (including AutoMS(n)), chromatogram display (overlaid), compound list and deconvolution results for each compound

DataAnalysis	Description
Display All Win All Analyses (L or P).layout†	Contents of all windows open for all data files selected. Viewing multiple data files is limited to the Chromatogram window.
Display All Win Selected Analyses (L or P).layout	Any windows displayed for analysis select in Analysis List, including Analysis Info, Chromatogram (all views) with legend, if overlaid
Display Selected Win All Analyses (L or P).layout	Contents of highlighted window displayed. Viewing multiple data files is limited to the Chromatogram window.
Display Selected Win Selected Analyses (L or P).layout	Contents of highlighted window contains analysis selected in Analysis List
Library Search Report - AutoMSn (P).layout	Analysis Info contains most important acquisition parameters (including AutoMS(n)), chromatogram display (overlaid), description of Fit, Rfit, and Purity calculations, compound identification results, compound mass spectra and library matching spectra
Selected Chromatogram Report (P).layout	Display of chromatogram in List view for analysis selected in Analysis List
Selected Mass Spectrum Report (P).layout	Contents of Mass Spectrum window corresponding to selected analysis is displayed. Mass Spectrum window contains data acquired in Trap Control (Acquisition > Save Profile Now).
Sensitivity Checkout Report (P).layout	Modified Cmpd Chrom Report 3R1C - MS (P).layout to represent S/N results for installation checkout
Single Mass Spec Decon Report (P).layout	Analysis Info contains important acquisition parameters, display of Mass Spectrum window and deconvolution results for spectrum
Quant Chrom Report ESTD (P).layout	Compilation of all data file Analysis Info contains most important Acquisition Parameters, displays of target compound ion chromatographic peaks, and Compound List information for quantitation batch using external standard reference.

DataAnalysis	Description
Quant Chrom Report ISTD (P).layout	Compilation of all data file Analysis Info contains most important Acquisition Parameters, displays of target compound ion chromatographic peaks, and Compound List information for quantitation batch using internal standard reference.
Quant Chrom+Spec Report ESTD (P).layout	Compilation of all data file Analysis Info contains most important Acquisition Parameters, displays of target compound ion chromatographic peaks and corresponding spectra, and Compound List information for quantitation batch using external standard reference.
Quant Chrom+Spec Report ISTD (P).layout	Compilation of all data file Analysis Info, most important Acquisition Parameters, displays of target compound ion chromatographic peaks and corresponding spectra, and Compound List information for quantitation batch using external standard reference.
Quant Summary Report ESTD (P).layout	Batch Info Quant Method Parameters contains the most important Acquisition Parameters, Sequence Table, tabulated Compound integration results with Calibration curves.
Quant Summary Report ISTD (P).layout	Batch Info, Quant Method Parameters contains the most important Acquisition Parameters, Sequence Table, tabulated Compound integration results with Calibration curves.

* (P) represents portrait mode. Although the layouts have been optimized for this paper orientation, they print in the landscape orientation as well. These layouts also print in A4 or Letter format. The report layouts are installed as part of the supplemental installation.

† For all Display reports, the windows available to open include Chromatogram, Mass Spectrum View, Compound Mass Spectra and Mass Spectrum windows.

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In this book

This book contains brief instructions and information to help you get started with your Agilent Ion Trap system. This book shows how to or where to get help to:

- Start and become familiar with the software.
- Prepare the instrument.
- Set up and run an acquisition method.
- Review data and identify compounds.
- Deconvolute and search protein spectra.
- Quantify compounds.
- Shut down or place the instrument in standby.

This book also contains a listing of new Ion Trap Software 6.2 features, shipped methods, and report layouts.

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